Parallel stochastic methods for exploring randomness in solar cell designs

A position paper prepared by

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I. Objective: Developing highly parallel stochastic methods in computational electromagnetics to explore designing spaces and calibrate the effect of disorder surfaces on achieving optimal light absorption of multilayered silicon solar cells, designed in Stanford Lab for maximal electrical carrier currents.

II. Extreme design complexity and computational challenges: Next generation solar cells employs *disordered surface* consisting of patterns of structural elements at nano-scales to enhance light absorption significantly over the broadband spectrum of sun lights. Experiments and simulations (Fig. 1) show that patterns with deterministic disorder outperform completely random and periodic structures [1][2][3]. The challenge is to find the optimal pattern efficiently with exascale computing technologies and algorithms.

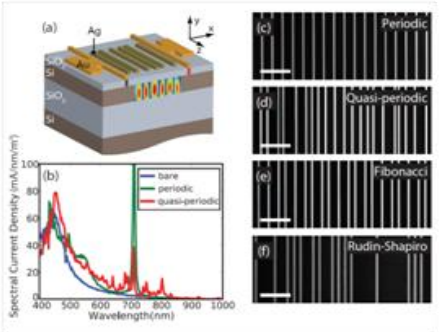

Fig. 1. Optimized disordered stripe arrays for enhanced light trapping in ultra-thin semiconductor layers [1].

As each structural degree freedom corresponds roughly to an area of $100\times100nm^2$ unit cell, a macroscopically area of $1cm^2$ on a solar cell gives $\mathbf{10^{10}}$ degrees of freedom. Efficient computational algorithms and optimization techniques are needed to bridge the macroscopic length scale of the cell, and the nano-scale of the underlying feature sizes, allowing engineers to create highly efficient solar cells by effectively *exploring the enormous design space*. This is one of most exciting scientific and engineering challenges where exascale computing can make a significant impact and become an enabling tool, and designing efficient solar cells will advance DOE's clean energy mission.

III. Parallel stochastic modeling methods: In engineering optimization, one often unavoidably has to search through large numbers of structures before the optimal solution is found. This is particularly true in nano-photonic design, where, due to wave interference and multiple scattering effects, variation in one part of a structure can have drastically impact on the overall optical properties of the structure. As one needs to explore large phase spaces efficiently, this presents a huge challenge for computational electromagnetic based engineering designs [5] and an opportunity for exascale computing.

Two parallel stochastic methods in computational electromagnetics will be developed to address this challenge for exascale computing: (a) a DtN (Dirichlet-to-Neumann) domain decomposition (**DtN-DD**) method [4] where each nano-photonic element is modeled by a DtN mapping, giving a parallel method to

study aperiodic configurations of structural elements; (b) a parallel stochastic boundary integral equation (**SBIE**) method using layered dyadic Green's functions and fast solvers for layered media.

- **DtN-DD**: The DtN-DD method is uniquely suited for optimization of large numbers of structures. The key idea is to seek a *local* basis that provides efficient representation of the electromagnetic field. Certainly, improving the efficiency of representation cuts down the computational cost. Moreover, having a local basis is important since in such a case a local adjustment of the structure, say, by changing a single element, can be very rapidly solved through low-rank adjustment, once the structure before the adjustment is solved. This dramatically simplifies the optimization process. In the field of complex photonic crystal simulations, the use of DtN technique has allowed us to search through *very large ensemble consisting of millions of samples* [1][4], a feat that is almost unheard of in previous photonic crystal simulations.

  At present, the DtN method is largely restricted to 2-D systems. A straightforward generalization of the existing DtN method to 3-D cases produces spurious modes due to the vector nature of the electromagnetic field. We will try to overcome this difficulty by a hybrid approach using some of the field representation techniques from the finite element and boundary element methods so a more judicious choice of the basis function can remove the spurious modes. Here, new mathematical treatments of the electromagnetic fields in 3-D nano-photonics structure will be very helpful in improving the robustness and convergence of the DtN-DD methods.

- **SBIE**: For each selection of the rough surface encountered in the solar cell design, a parallel method for BIEs of the form

$$i\omega\mu\vec{n}\times\int_S \ddot{G}(\vec{r},\vec{r}')\cdot\vec{J}(\vec{r}')ds' = \vec{n}\times\vec{E}^{inc}(\vec{r}),$$

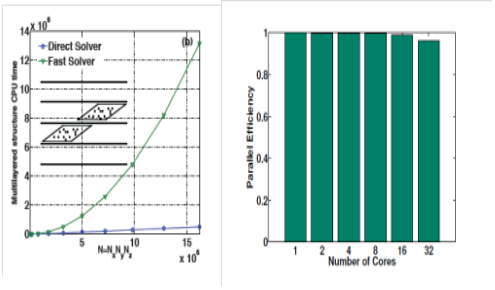

Fig. 2 (left) Speedup and (right) parallel scalability of Helmholtz integral operator in layered media for randomly distributed 1.5 mil. sources [7].

$\vec{E}^{inc}$ as the incident light source, uses a quadrature based fast evaluation of the dyadic Green's in the form of $\bar{G}(\rho;z,z') = \sum_{s=1}^{N_q}\Gamma_s J_0(\rho k_\rho^s)F(z,z';k_\rho^s)$. Here the number of quadrature points N_q in a contour in the spectral space is minimized by using a window-based filtering technique developed in our group [6] and specially designed quadrature formula based on the behavior of surface wave poles for wave propagations in layered media [7]. For each k_ρ^s, the Hankel kernel will be implemented by a fast tree code. Fig. 2 (left) shows [7] the speed up of the integral operator matrix for the scalar Helmhotlz integral operator in a matrix-vector product, compared with a direct product, and Fig. 2 (right) shows the scalability in a multi-nodes workstation. Further development of this fast solver for Maxwell fields in layered structures will be done. We will also consider other algorithmic issues for the SBIE, including succinct representations of rough surfaces [8][9], model reductions, and fast parameter space search, etc.

IV. References:

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